ORNL Tools and Capabilities for Analysis of the Liquid-Salt VHTR

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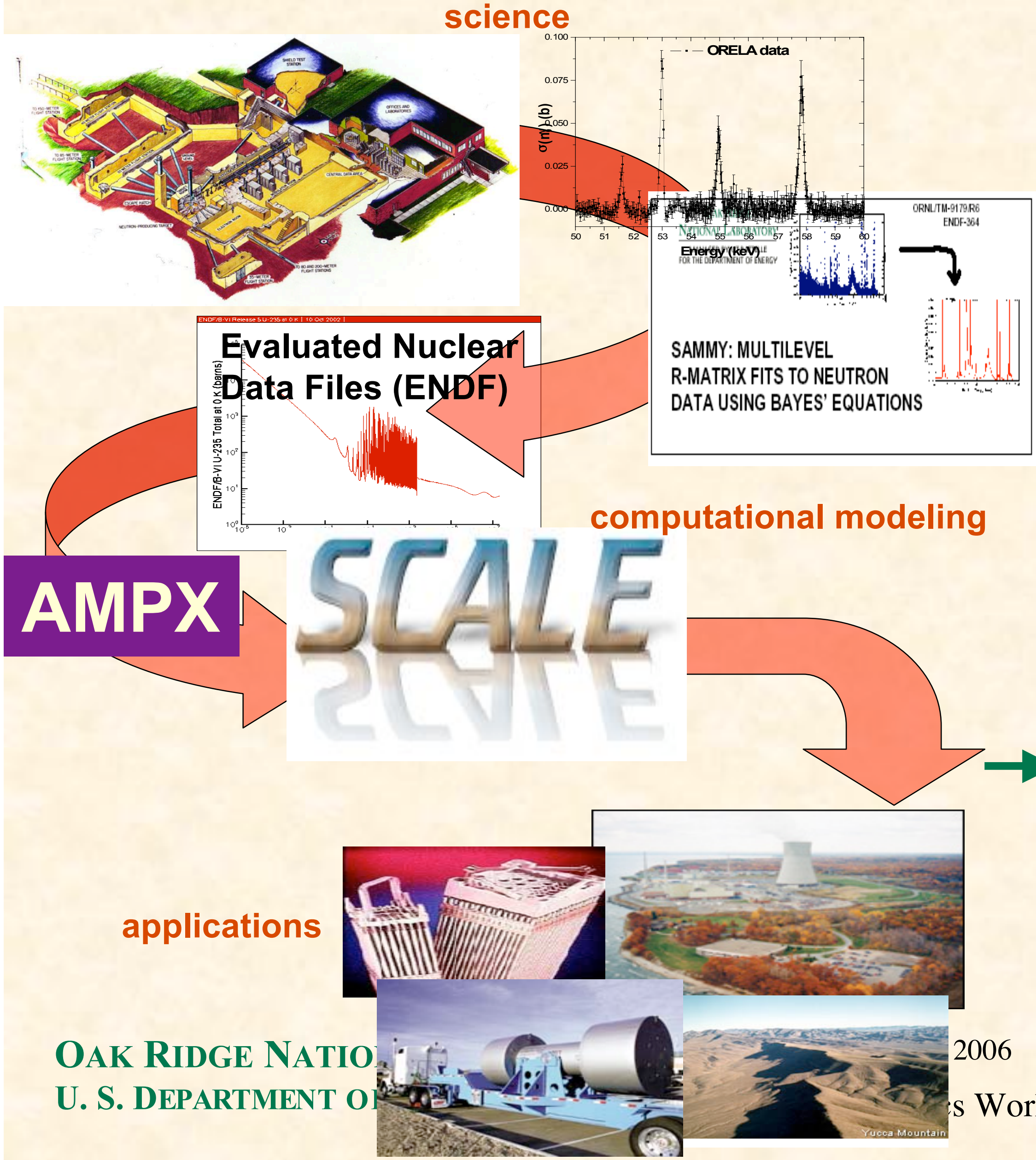
Nuclear Science & Technology Division

Outline

- The SCALE Code System
  - Description and recent developments
- The Liquid Salt-cooled VHTR Challenges
  - ~~Basic Design of the System~~ – Thank you Jim.
  - Primary Issues and Challenges
- Results from Salt Coolant Studies
- Results from 3-D Neutron Transport Analyses
- Conclusions
  - Applicability of ORNL Tools to AFCI/Gen-IV Analyses
  - Recommended improvements for greater applicability

SCALE @ ORNL: Science to Applications



Interface **science** (the basic physics of cross-section measurements), **computational modeling** (SCALE), and **applications** expertise to support evaluation and resolution of nuclear engineering and safety issues.

- Cross-section processing
- Criticality safety
- Radiation protection and shielding
- Reactor physics
- SNF/waste characterization (e.g., inventory, decay heat, radiation source and spectra)

Resonance Self-Shielding in SCALE: Accurate solutions need accurate data

- BONAMI: **Bondarenko Method**

  for unresolved resonance range

- NITAWL: **Nordheim Integral Method**

  for resolved resonance range (ENDF/B-V and earlier)

- CENTRM: **Continuous ENergy TRansport Module**

  for resolved resonance range (all libraries: ENDF/B-VI)

  - **Performs 1-D S_n calculation for continuous-energy neutron spectra using with Point-Wise nuclear data**
  - **Processes problem-dependent multigroup XS's using Point-Wise nuclear data and flux spectrum**

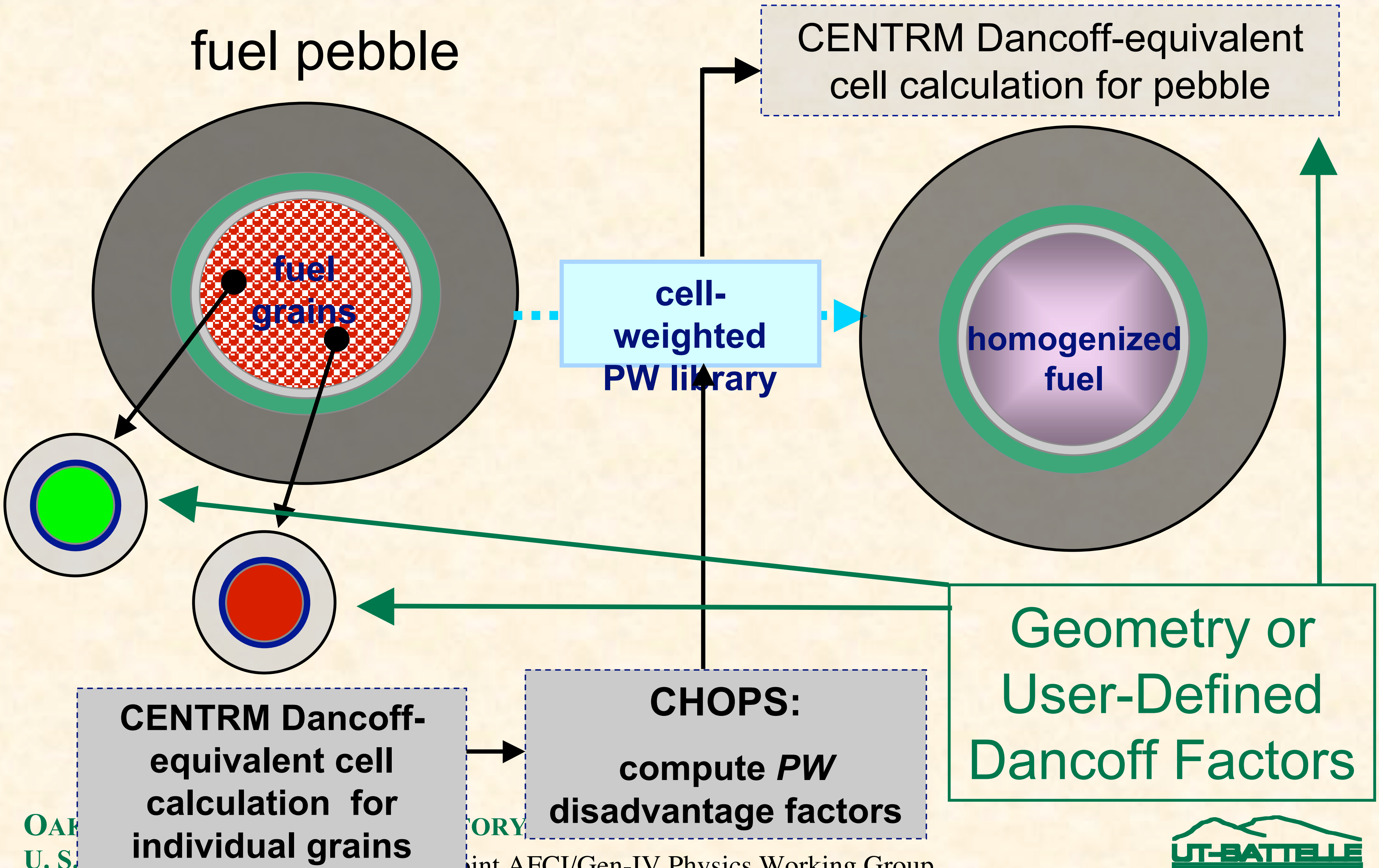
CENTRM Expands Traditional Resolved Resonance Self-Shielding Capabilities

- **ENDF/B-VI: Level-level interference effects; Reich-Moore Formalism**
- **Spatial Effects: Space-dependent self-shielding**
  - **absorber lump in absorber solution**
  - **“rim” effects in fuel pins**
- **Multiple Isotopes: Accounts for resonance overlap effects**
- **Anisotropic scatter and leakage impacts are included**
- **Current-weighting: Optional use of current to weight the cross sections**
- **Inelastic scattering: treatment for a problem-dependent spectra**

New and Improved

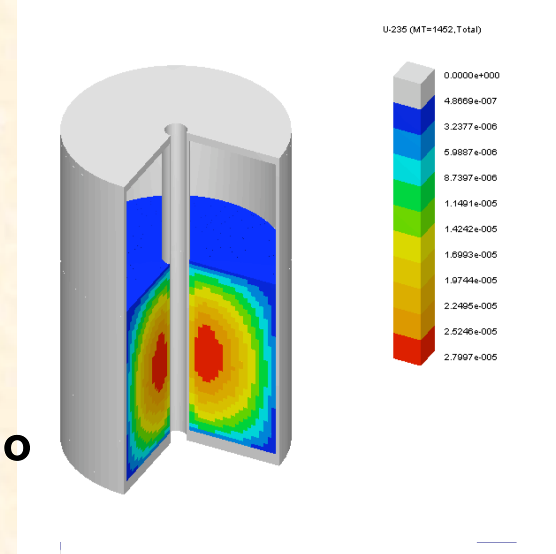
- **Improved elastic removal for structural and moderator materials**
- **PW thermal spectra: includes S(a,b) scattering to treat upscatter effects**
- **New and improved treatment of heterogeneities**
  - **Monte Carlo computation of Dancoff factors**
  - **Inverse procedure to obtain Dancoff-equivalent unit cell for CENTRM**
- **Double heterogeneity calculation**

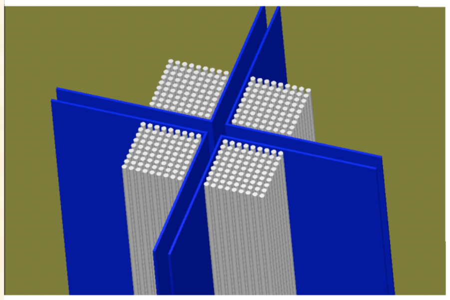
SCALE Double Heterogeneity Method



SCALE Stochastic Transport Methods

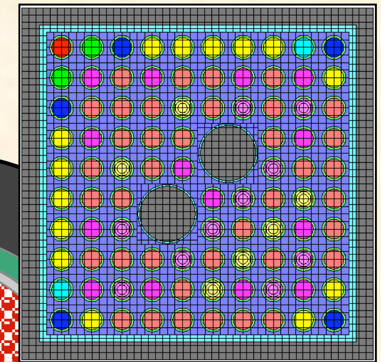
- **KENO-5 and KENO-VI multi-group Monte Carlo codes**
  - Developed for criticality safety applications
  - Much faster than continuous energy
  - Now integrated with TRITON for depletion
- **Continuous Energy KENO**
  - Currently under development
  - Provides the rigor of continuous energy Monte Carlo
- **MORSE/MONACO Monte Carlo Shielding Code**
  - Advanced variance reduction
- **A Single Consistent Geometry**
  - SCALE Generalized Geometry Package (SGGP) being adopted for all ORNL codes
  - Easily switch from NEWT to KENO-VI to CE-KENO

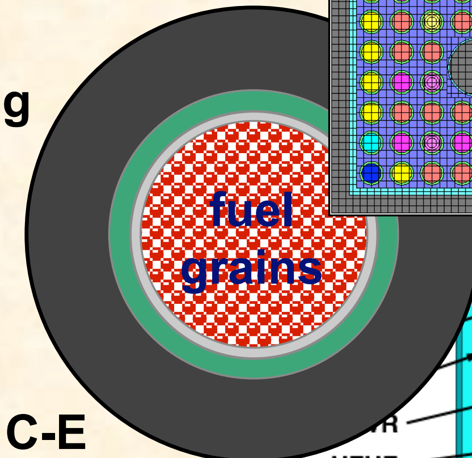


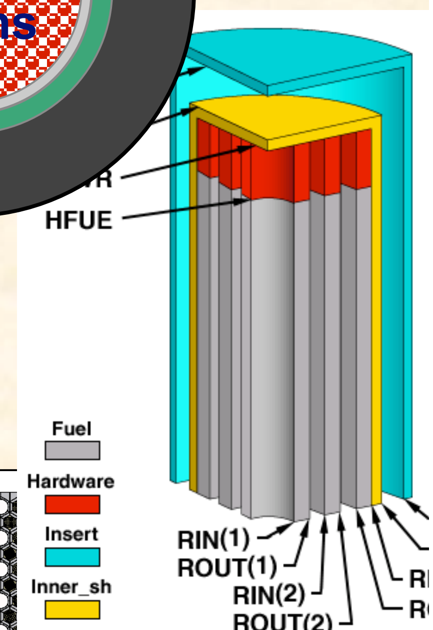


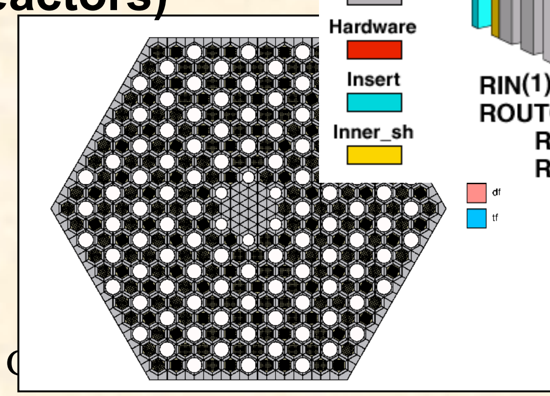
SCALE Deterministic Transport Methods

- **CENTRM**
  - 1-D, source-driven, continuous-energy
  - For problem-dependent resonance processing
- **XSDRNPM**
  - 1-D, WDD, multi-group
  - Forward/adjoint with a host of uses
- **GEMINEWTRN**
  - 2-D arbitrary polygonal mesh, source-driven, C-E
  - For problem-dependent resonance processing
- **NEWT**
  - 2-D arbitrary polygonal mesh, multi-group
  - Forward/adjoint solutions for all analyses (reactors)
- **TORT**
  - 3-D orthogonal mesh, multi-group
  - For all analyses, widely-used in shielding









ORIGEN-S: Irradiation and decay simulation code

- Irradiation and decay simulation code
- Explicit simulation of 1484 unique nuclides (1946 nuclides in database)
  - 129 actinides
  - 1119 fission products
  - 698 structural activation materials
  - Other depletion codes typically track a minimum subset of isotopes that are important for reactivity
- Detailed radionuclide compositions
- Decay heat sources (neutron/photon), including energy spectra
- Radio-toxicity
- One of few codes available with comprehensive isotopic characterization of fuel over time scale of <u>seconds to millennia</u>
  - Accident analyses
  - Storage and handling
  - Transportation
  - Disposal or reprocessing
  - Repository analysis (storage, migration, dose assessment)

History of ORIGEN Code Development

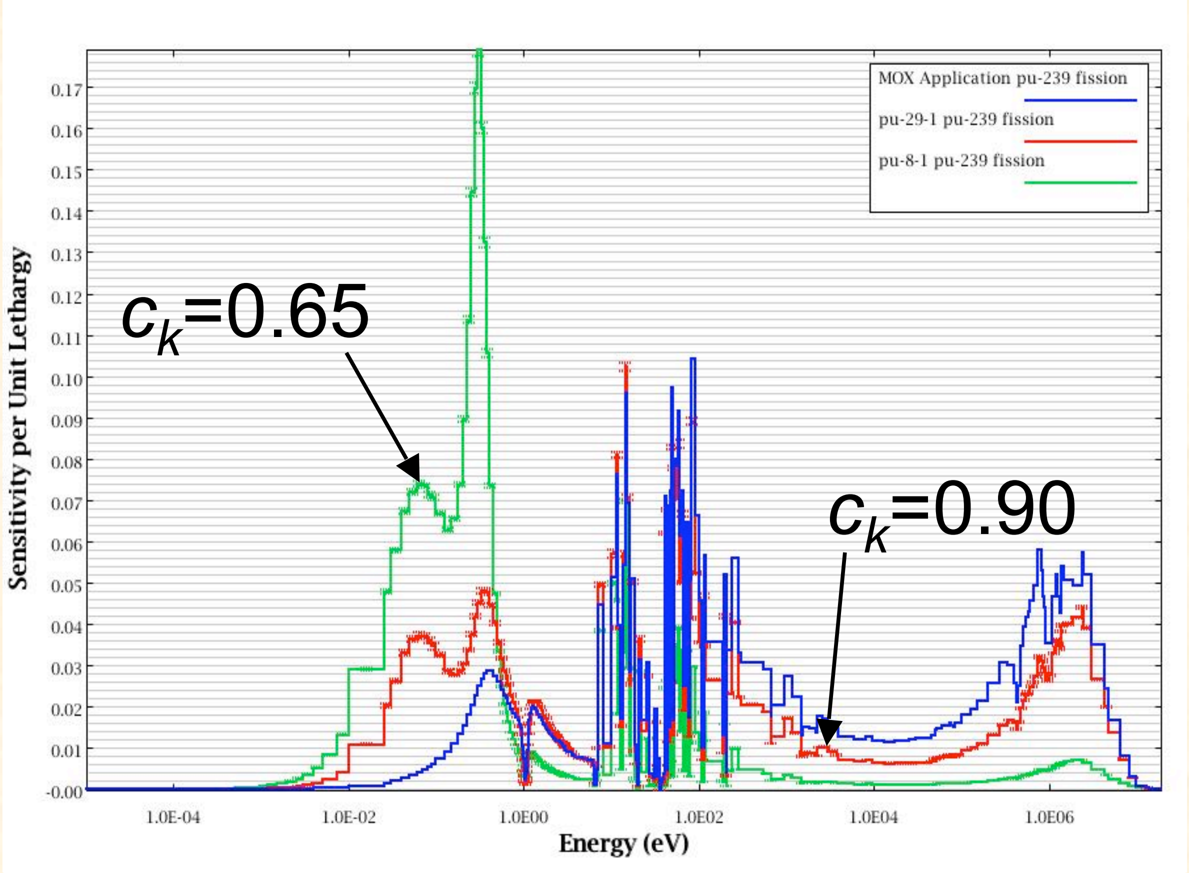
ORIGEN (1973)

ORIGEN-S	ORIGEN2
SCALE Module (1982)	User friendly input (1980)
QA configuration control	Standalone code in widespread use
Designed with modular data interface	Very limited libraries, data hard-wired
Active development and support by DOE & NRC	Obsolete nuclear data
Modern nuclear data	No neutron spectra
Extensive validation	No code and data development
Comprehensive radiation sources	Not supported at ORNL
Graphical Windows Interface	No QA activities

TSUNAMI: Tool for S/U Analysis with XSDRN (1-D) and KENO-VI (3-D)

- **Determination of critical experiment benchmark applicability to nuclear criticality safety analyses**
- **The design of critical general physics experiments (GPE)**
- **The estimation of computational biases and uncertainties for the determination of safety subcritical margins**

^{239}Pu Fission Sensitivity Profiles: Sensitivity of k_{eff} to cross-section



A few TSUNAMI Tools within SCALE

TSUNAMI-3D (Tools for Sensitivity and Uncertainty Analysis Methods Implementation – 3 Dimensional)

KENO Monte Carlo computes 3-D system sensitivity of k_{eff} and reactivity responses to neutron cross sections for individual:

- Nuclide(s)
- Reaction(s)
- Energy(ies)

$$\frac{\Delta_k}{k_{eff}} \Big/ \frac{\Delta_\Sigma}{\Sigma}$$

JavaPEÑO (Java Plots, Especially Nice Output)

Java ® interactive two-dimensional plotting package

Reads sensitivity data files from TSUNAMI-3D output

TSUNAMI-IP (Tools for Sensitivity and Uncertainty Analysis Methods Implementation – Indeces and Parameters)

Processes output from TSUNAMI-3D to generate relational parameters and indeces for:

Estimating the degree of similarity between two fissionable material systems

Primary physics issues & challenges associated with the LS-VHTR

- Coolant
  - Voiding
    - What happens to the reactivity if we lose coolant?
    - Does it matter when other changes are accounted for?
  - Activation
    - How does it change due to activation?
    - How do transmutation products effect refueling and long term storage?
  - Cost and Handling
    - Thermo-physical properties
    - Neutronic-activation properties during operation

- Refueling
  - How do we refuel above 350 ^{o}C with possibly activated coolant?
  - Where do we store 2-3 times as many blocks as the VHTR

- Core and Fuel Block Design
  - Optimization varies with salt choice, and design parameters
    - Enrichment, discharge burnup, number and length of cycles
    - Density and temperature coefficients
  - Refueling considerations

Initial Salt Coolants for the LS-VHTR

Alkali Fluorides	*ZrF_4 – salts*	*BeF_2 – salts*
	LiF-ZrF_4 (51-49) 509°C NaF-ZrF_4 500°C	
LiF-KF (1) 492°C LiF-RbF (44-56) 470°C		
LiF-NaF-KF (46.5-11.5-42) 454°C		LiF-BeF_2 (67-33) 460°C
LiF-NaF-RbF (42-6-52) 435°C	LiF-NaF-ZrF_4 (26-37-37) 436°C	LiF-BeF_2-ZrF_4 (64.5-30.5-5) 428°C
	RbF-ZrF_4 (58-42) 410°C (52-48) 390°C	
	KF-ZrF_4 (58-42) 390°C	
		NaF-BeF_2 (57-43) 340°C LiF-NaF-BeF_2 (31-31-38) 315°C

Reactivity insertion from coolant voiding – this is not a LWR

- **Rapid loss of coolant w/o temp. change unlikely**
  - Pool-type design @ atmospheric pressure
  - High boiling point (>1400 ^{o}C): 400-700 ^{o}C above nominal
  - Positive CDC (CVR) is politically sensitive

- **If coolant heats up, so can graphite and fuel**
  - Power driven transient: DFuel > DCoolant
    - If Doppler is as negative as CVR is positive… no problem
  - Temperature driven transient: DCoolant > DFuel
    - How much DFuel is required to offset a DCoolant?
    - Safety Ratio ~ FTC / CDC

- **Reactor design effects these properties**

Estimator for Salt Coolant Physics

Parameters	Value	Units
Cycle Length	1.5	Years
Cycles per Core	2	Number of Batches
Refueling Length	20	Days
Coolant Fraction	7	Volume % of Coolant in the Fuel Block
^{6}Li Content	0.005	Weight % of ^{6}Li in Lithium
Poison Content	0	mg/cm^3 Er_2O_3 in the Fuel Compact Matrix

Salt	Eutectic	^{235}U Enrichment	Burnup	Coolant Void Ratio	Total Coolant Temp. Coef.	Safety Ratio	Isothermal Temperature Coefficient
	atom%	wt%	MW-d/kgHM	Dollars	Dollars per 100 °C	%	Dollars per 100 °C
LiF_BeF_2	(67_33)	**14.8**	158.3	$0.26	$0.00	0.6%	**-$0.48**
NaF_BeF_2	(57_43)	**16.1**	158.3	$2.59	$0.07	23.5%	**-$0.22**
$LiF\_NaF\_ZrF_4$	(26_37_37)	**16.3**	158.3	$2.72	$0.09	28.3%	**-$0.22**
NaF_ZrF_4	(59.5_40.5)	**16.6**	158.3	$3.22	$0.10	43.1%	**-$0.14**
$NaF\_RbF\_ZrF_4$	(33_23.5_43.5)	**17.4**	158.3	$4.25	$0.13	97.0%	$0.00

Salt	Eutectic	Coefficients of Reactivity					
		Coolant			Non-Coolant		
		Temperature	Density	Total	Fuel	Graphite	Total
	atom%		Dollars per 100 °C			Dollars per 100 °C	
LiF_BeF_2	(67_33)	$0.00	$0.01	**$0.00**	-$0.43	-$0.05	**-$0.48**
NaF_BeF_2	(57_43)	$0.00	$0.06	**$0.07**	-$0.38	$0.09	**-$0.28**
$LiF\_NaF\_ZrF_4$	(26_37_37)	$0.00	$0.08	**$0.09**	-$0.38	$0.07	**-$0.30**
NaF_ZrF_4	(59.5_40.5)	$0.00	$0.11	**$0.10**	-$0.36	$0.12	**-$0.24**
$NaF\_RbF\_ZrF_4$	(33_23.5_43.5)	$0.00	$0.15	**$0.13**	-$0.33	$0.20	**-$0.13**

Estimator for Salt Coolant Physics

Parameters	Value	Units
Cycle Length	1.5	Years
Cycles per Core	2	Number of Batches
Refueling Length	20	Days
Coolant Fraction	7	Volume % of Coolant in the Fuel Block
^{6}Li Content	0.005	Weight % of ^{6}Li in Lithium
Poison Content	5	mg/cm^3 Er_2O_3 in the Fuel Compact Matrix

Salt	Eutectic	^{235}U Enrichment	Burnup	Coolant Void Ratio	Total Coolant Temp. Coef.	Safety Ratio	Isothermal Temperature Coefficient
	atom%	wt%	MW-d/kgHM	Dollars	Dollars per 100 °C	%	Dollars per 100 °C
LiF_BeF $_2$	(67_33)	**15.1**	158.3	**-$0.13**	**-$0.09**		**-$2.43**
NaF_BeF $_2$	(57_43)	**16.4**	158.3	$2.32	**-$0.01**		**-$2.16**
LiF_NaF_ZrF $_4$	(26_37_37)	**16.5**	158.3	$2.78	$0.04	2.0%	**-$2.13**
NaF_ZrF $_4$	(59.5_40.5)	**16.9**	158.3	$3.30	$0.06	3.0%	**-$2.04**
NaF_RbF_ZrF $_4$	(33_23.5_43.5)	**17.7**	158.3	$4.78	$0.11	5.3%	**-$1.89**

Salt	Eutectic	Coefficients of Reactivity					
		Coolant			Non-Coolant		
		Temperature	Density	Total	Fuel	Graphite	Total
	atom%		Dollars per 100 °C			Dollars per 100 °C	
LiF_BeF $_2$	(67_33)	-$0.09	$0.00	**-$0.09**	-$0.89	-$1.47	**-$2.35**
NaF_BeF $_2$	(57_43)	-$0.07	$0.06	**-$0.01**	-$0.83	-$1.32	**-$2.15**
LiF_NaF_ZrF $_4$	(26_37_37)	-$0.05	$0.09	**$0.04**	-$0.84	-$1.34	**-$2.17**
NaF_ZrF $_4$	(59.5_40.5)	-$0.04	$0.11	**$0.06**	-$0.82	-$1.29	**-$2.10**
NaF_RbF_ZrF $_4$	(33_23.5_43.5)	-$0.04	$0.15	**$0.11**	-$0.79	-$1.21	**-$1.99**

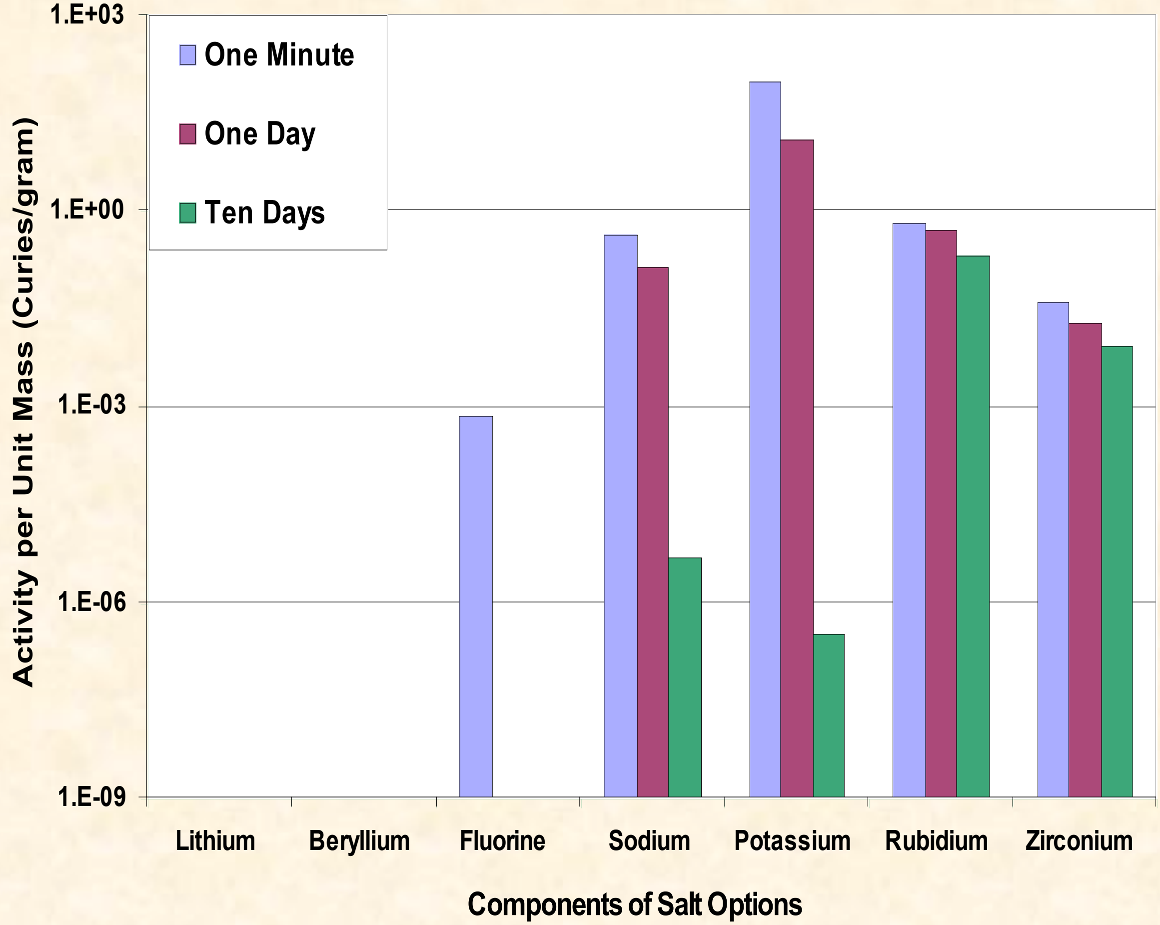
Estimator for Salt Coolant Physics

Parameters	Value	Units
Cycle Length	1.5	Years
Cycles per Core	2	Number of Batches
Refueling Length	20	Days
Coolant Fraction	15	Volume % of Coolant in the Fuel Block
^{6}Li Content	0.005	Weight % of ^{6}Li in Lithium
Poison Content	5	mg/cm^3 Er_2O_3 in the Fuel Compact Matrix

Salt	Eutectic	^{235}U Enrichment	Burnup	Coolant Void Ratio	Total Coolant Temp. Coef.	Safety Ratio	Isothermal Temperature Coefficient
	atom%	wt%	MW-d/kgHM	Dollars	Dollars per 100 °C	%	Dollars per 100 °C
LiF_BeF $_2$	(67_33)	**16.2**	158.3	**-$0.67**	**-$0.19**		**-$2.30**
NaF_BeF $_2$	(57_43)	**18.7**	158.3	$4.51	**-$0.04**		**-$1.70**
LiF_NaF_ZrF $_4$	(26_37_37)	19.4	158.3	$5.72	$0.08	4.4%	**-$1.68**
NaF_ZrF $_4$	(59.5_40.5)	**20.0**	158.3	$6.84	$0.12	7.6%	**-$1.46**
NaF_RbF_ZrF $_4$	(33_23.5_43.5)	**22.0**	158.3	$10.27	$0.21	16.1%	**-$1.10**

Salt	Eutectic	Coefficients of Reactivity					
		Coolant			Non-Coolant		
		Temperature	Density	Total	Fuel	Graphite	Total
	atom%		Dollars per 100 °C			Dollars per 100 °C	
LiF_BeF $_2$	(67_33)	-$0.19	-$0.01	**-$0.19**	-$0.88	-$1.23	**-$2.10**
NaF_BeF $_2$	(57_43)	-$0.15	$0.06	**-$0.04**	-$0.76	-$0.91	**-$1.66**
LiF_NaF_ZrF $_4$	(26_37_37)	-$0.10	$0.17	**$0.08**	-$0.78	-$0.98	**-$1.76**
NaF_ZrF $_4$	(59.5_40.5)	-$0.10	$0.11	**$0.12**	-$0.73	-$0.85	**-$1.58**
NaF_RbF_ZrF $_4$	(33_23.5_43.5)	-$0.10	$0.15	**$0.21**	-$0.66	-$0.66	**-$1.31**

Activation & Transmutation Effect Refueling and Storage Options



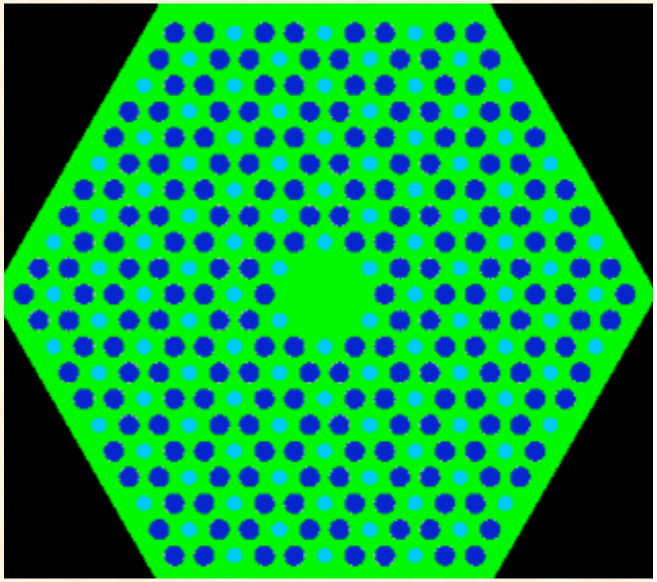
	Activity after Ten Years of Decay								
	All Radiation (Ci/g_coolant)								
Isotope	Radiation (keV)	Effective T1/2	Lithium	Beryllium	Fluorine	Sodium	Potassium	Rubidium	Zirconium
Be-10	Electron	1.5 Million Years		2.E-07					
Na-22	Positron	3 Years				2.E-09			
Cl-36	Electron	300 Thousand Years					**1.E-06**		
K-40	Gamma (1.5)	1 Billion Years					4.E-08		
Rb-87	Electron	50 Billion Years						2.E-08	
Zr-93	Gamma (0.03)	1.5 Million Years							4.E-07
Nb-93m	Gamma (0.03)	1.5 Million Years							3.E-07
Ten Years (All Radiation)			0.E+00	2.E-07	0.E+00	2.E-09	**1.E-06**	2.E-08	7.E-07

Cost and Handling Challenges of Salts

- High freezing points (~350-500 ^{o}C)
  - Challenge refueling and maintenance outages
- High vapor pressure
  - For some salts
- Beryllium toxicity
  - If a BeF_2 salt is used
- High cost of lithium enrichment
  - If a LiF salt is used
- Limited experience
  - With some salts, like those with RbF
- Enrichment penalty due to parasitic capture
  - ^{6}Li, K, Zr

Axial-layering of Er_2O_3 poison can significantly reduce the CVR

Cooled Eigenvalue	1.259	1.250	1.250	1.250
Voided Eigenvalue	1.265	1.240	1.241	1.241
CVR ($)	$0.54	-$0.94	-$0.83	-$0.88
1	Reflector	Reflector	Reflector	Reflector
2	Fuel	Poison	Poison	Poison
3	Fuel	Poison	Poison	Fuel
4	Fuel	Fuel	Fuel	Fuel
5	Fuel	Fuel	Fuel	Poison
6	Fuel	Poison	Poison	Poison
7	Fuel	Poison	Fuel	Fuel
8	Fuel	Poison	Poison	Poison
9	Fuel	Fuel	Fuel	Poison
10	Fuel	Fuel	Fuel	Fuel
11	Fuel	Poison	Poison	Fuel
12	Fuel	Poison	Poison	Poison
13	Reflector	Reflector	Reflector	Reflector

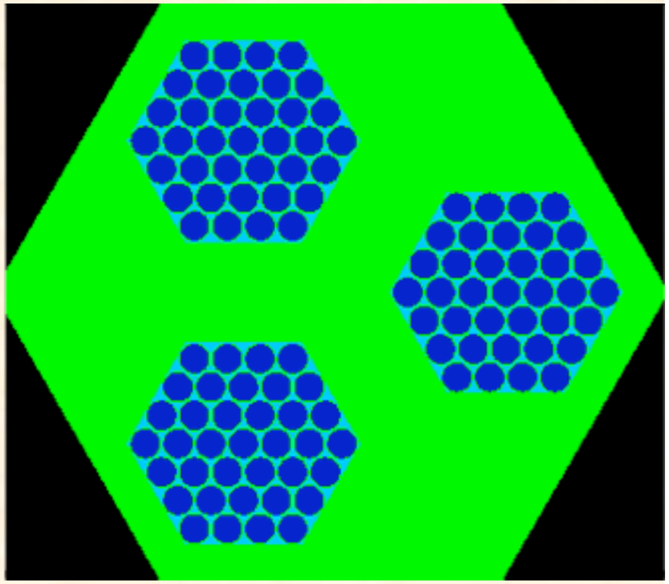


Refueling is the major issue today

- **The challenge:**
  - Very hot: > 350 ^{o}C
  - Many more fuel blocks than the VHTR
    - 600 MWt VHTR = 1020 blocks
    - 2400 MWt LS-VHTR = 2650 blocks
  - Coolant may have a high dose rate

- **Solutions:**
  - Pebble Bed – very high coolant fraction
  - Robotics – already expected with VHTR
  - Larger blocks – possibly feasible?
  - Assemblies – industry approves

- **Are assembly designs feasible?**
  - Full-length graphite-clad rods, clustered together like an LWR fuel assembly
  - Passive safety is not a problem
    - Natural circulation of salt
    - Not just graphite conduction
  - More reuse of nuclear-grade graphite
  - Enrichment/poison grading is required



The assembly design: similar to the ACR-700, with less uncertainty

This can now be done directly using a TSUNAMI sequence.

	Base Block	Assembly without Enrichment Grading	Assembly with Enrichment Grading	ACR-700
k_{cool}	1.242	1.268	1.260	1.257
Δp	-\$2.05	-\$1.19	-\$1.38	-\$10.30
Δf	\$1.40	\$1.21	\$1.08	\$5.71
$\Delta \varepsilon$	\$0.90	\$0.88	\$1.02	\$5.11
$\Delta \eta$	-\$0.17	-\$0.16	-\$0.69	-\$0.78
CVR	\$0.08	\$0.74	\$0.03	-\$0.26
σ	\$0.01	\$0.01	\$0.01	

Conclusions

- **SCALE:**
  - Many qualified, easy to use tools for nuclear analysis
  - Rigorous and independent models ideal for benchmarking
  - Has been used for a wide variety of systems:
    - Reactor analysis, experiment design, shielding, crit. safety, etc.
  - Many tools are directly applicable to Gen-IV systems and the Advanced Fuel Cycle Initiative
- **LS-VHTR:**
  - Salt-coolant alternative for the VHTR
  - Coolant voiding:
    - Previously primary issue
    - Has been shown to be of little significance for many salts
  - Refueling:
    - Very high temperature with many fuel blocks
    - Very challenging: currently the primary issue
    - Several options have been/are being considered

How can ORNL help Gen-IV and AFCI?

- **Multi-group cross sections:**
  - **Accurate, problem-dependent MG cross sections**
  - **3-D depletion of doubly-heterogeneous systems**
- **Isotopic analysis:**
  - **Benchmarking current tools (ORIGEN2) w/ SCALE (ORIGEN-S)**
  - **ORIGEN-S replacement for ORIGEN2 applications**
- **System/experiment analyses:**
  - **Benchmarking current system analyses with SCALE**
  - **S/U analysis of isotopics and reactivity parameters for a system**
  - **Applicability assessment of experiments to reactor systems**
  - **Bias and uncertainty analysis of experiments**
- **Anything else?**